

Sample name: **D07**
Assay name: **UV-metric psKa**
Assay ID: **17J-07003**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 2:51:21 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

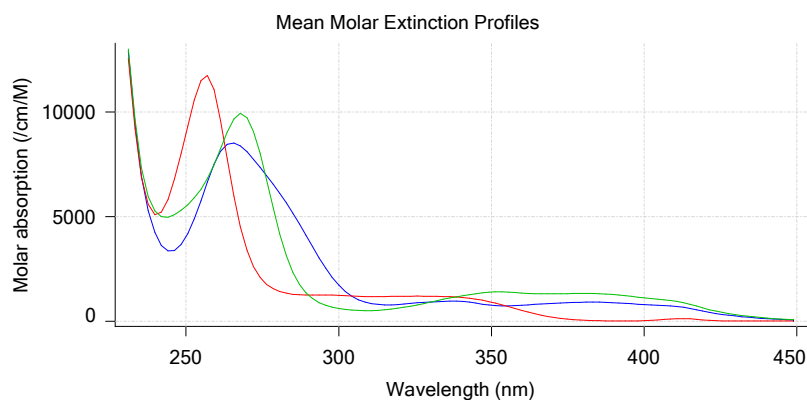
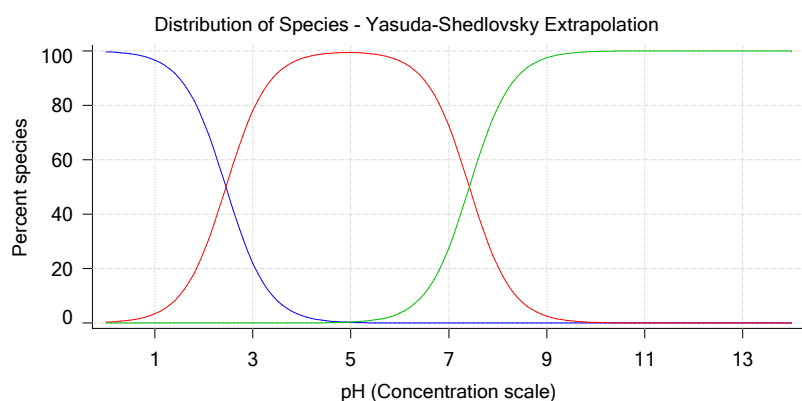
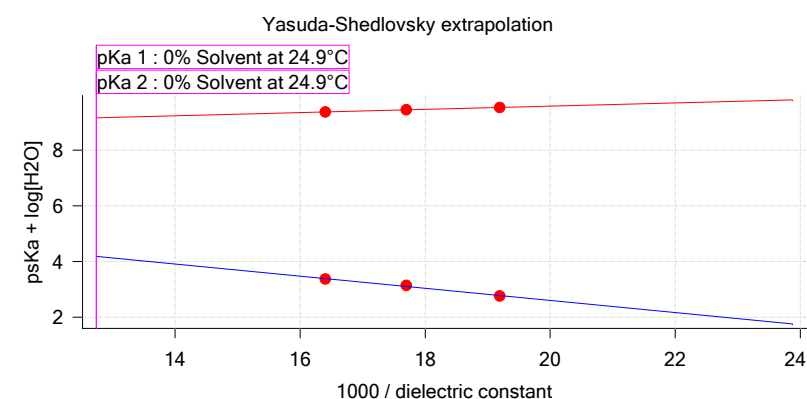
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	2.45	±0.10	6.98	-218.9668	0.9925	0.166 M	24.9°C
Yasuda-Shedlovsky	7.42	±0.03	8.43	57.7140	0.9916	0.166 M	24.9°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H ₂ O]	Ionic strength	Temperature	psKa 1	psKa 2
17J-07003 Points 4 to 69	59.07 %	Up	UV-metric pKa	52.1	19.6 M	0.157 M	24.9°C	✓ 1.47	✓ 8.24
17J-07003 Points 71 to 140	49.72 %	Up	UV-metric pKa	56.5	24.6 M	0.167 M	24.9°C	✓ 1.75	✓ 8.07
17J-07003 Points 142 to 212	40.08 %	Up	UV-metric pKa	61.0	30.0 M	0.174 M	24.9°C	✓ 1.90	✓ 7.89

Graphs



UV-metric psKa Titration 1 of 3 17J-07003 Points 4 to 69

Results

pKa 1 **1.47**
pKa 2 **8.24**
RMSD **0.004 0.002 0.005**
Chi squared **0.0432**
PCA calculated number of pKas **6**
Average ionic strength **0.157 M**
Average temperature **24.9°C**
Analyte concentration range **81.2 µM to 76.3 µM**
Methanol weight % **59.1 %**
Dielectric constant **52.1**
Water concentration **19.6 M**

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Experiment start time: **10/7/2017 2:51:21 AM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T311053**

Results (continued)

Number of pKas source **Predicted**
 Wavelength clipping **230.0 nm to 450.0 nm**
 pH clipping **1.462 to 12.542**

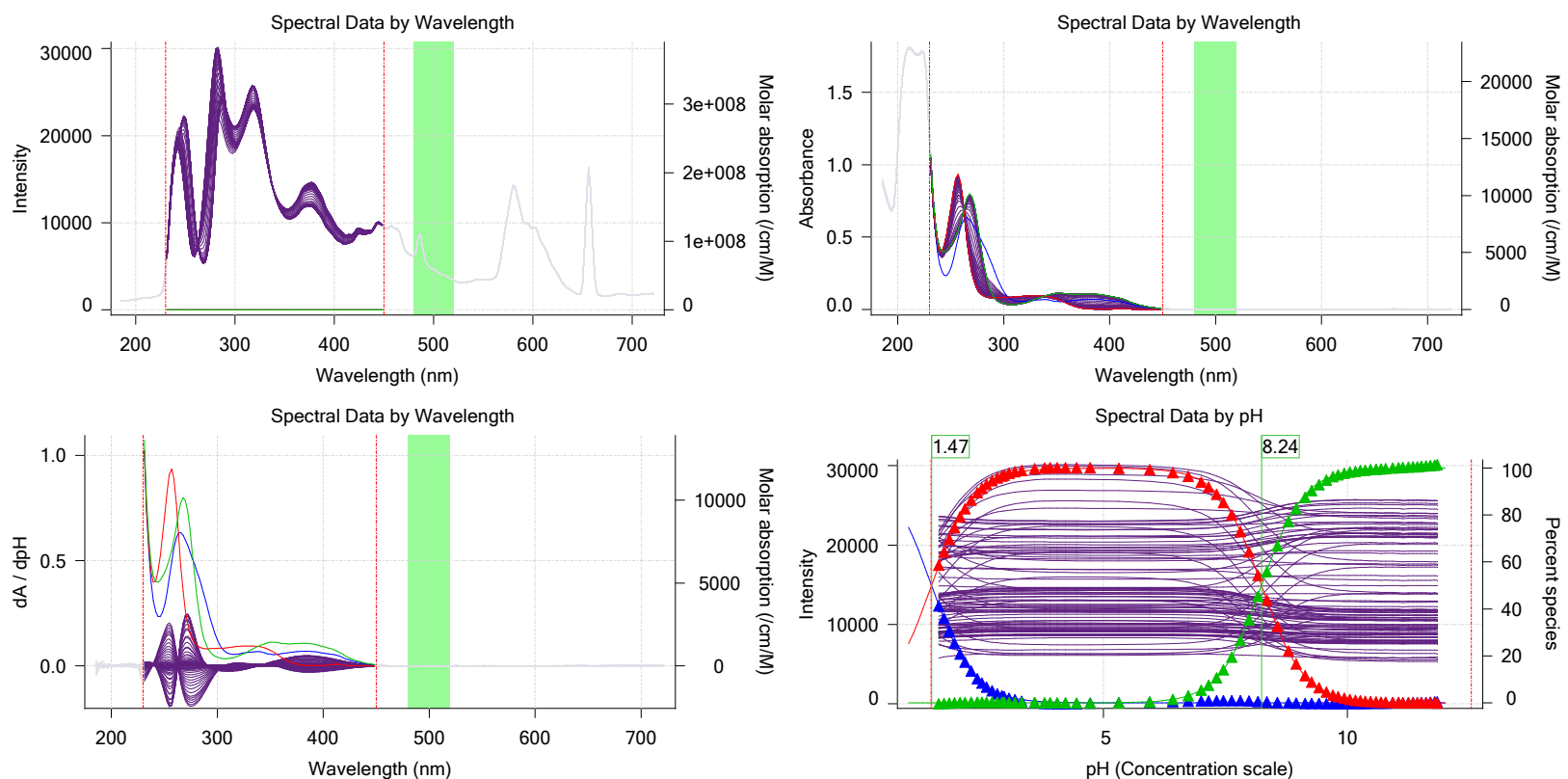
Warnings and errors

Errors None
 Warnings PCA calculation disagrees with predicted number of pKas

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

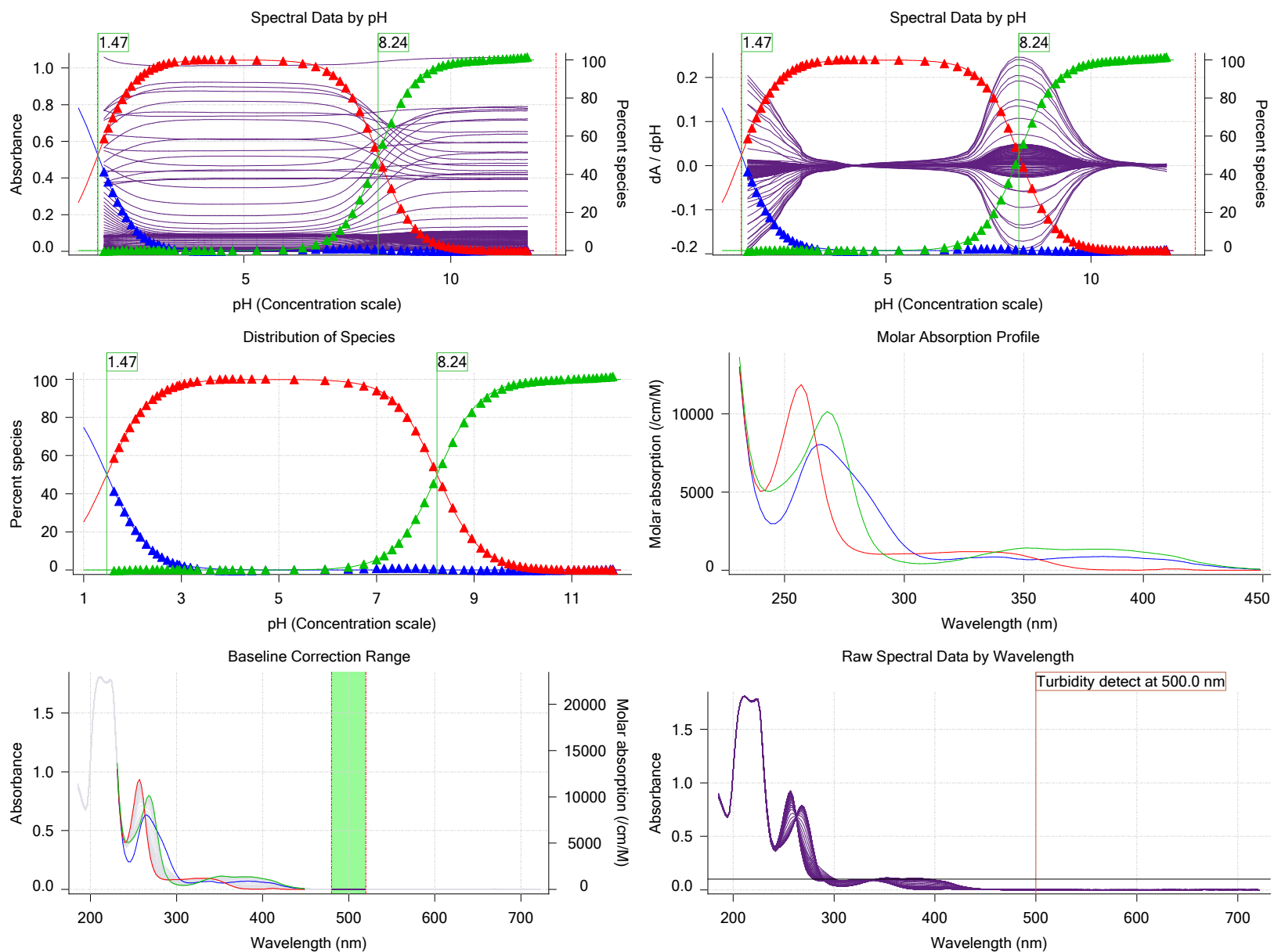
Graphs



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Experiment start time: **10/7/2017 2:51:21 AM**
 Analyst: **Dorothy Levorse**
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Graphs (continued)



UV-metric psKa Titration 2 of 3 17J-07003 Points 71 to 140

Results

pKa 1 **1.75**
 pKa 2 **8.07**
 RMSD **0.005 0.007 0.005**
 Chi squared **0.0506**
 PCA calculated number of pKas **6**
 Average ionic strength **0.167 M**
 Average temperature **24.9°C**
 Analyte concentration range **69.4 µM to 65.5 µM**
 Methanol weight % **49.7 %**
 Dielectric constant **56.5**
 Water concentration **24.6 M**

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Experiment start time: **10/7/2017 2:51:21 AM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T311053**

Results (continued)

Number of pKas source **Predicted**
 Wavelength clipping **230.0 nm to 450.0 nm**
 pH clipping **1.495 to 12.539**

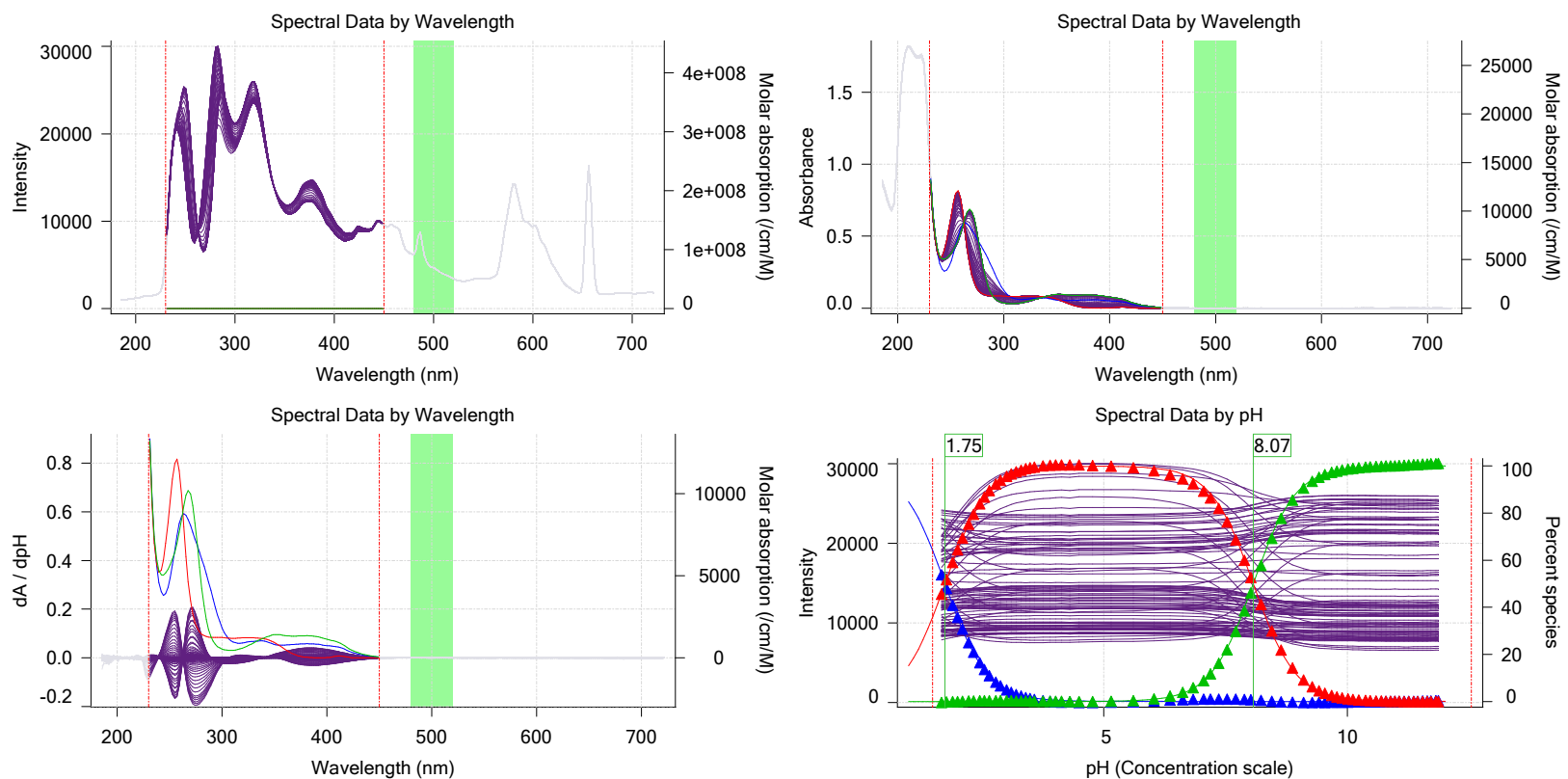
Warnings and errors

Errors **None**
 Warnings **PCA calculation disagrees with predicted number of pKas**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

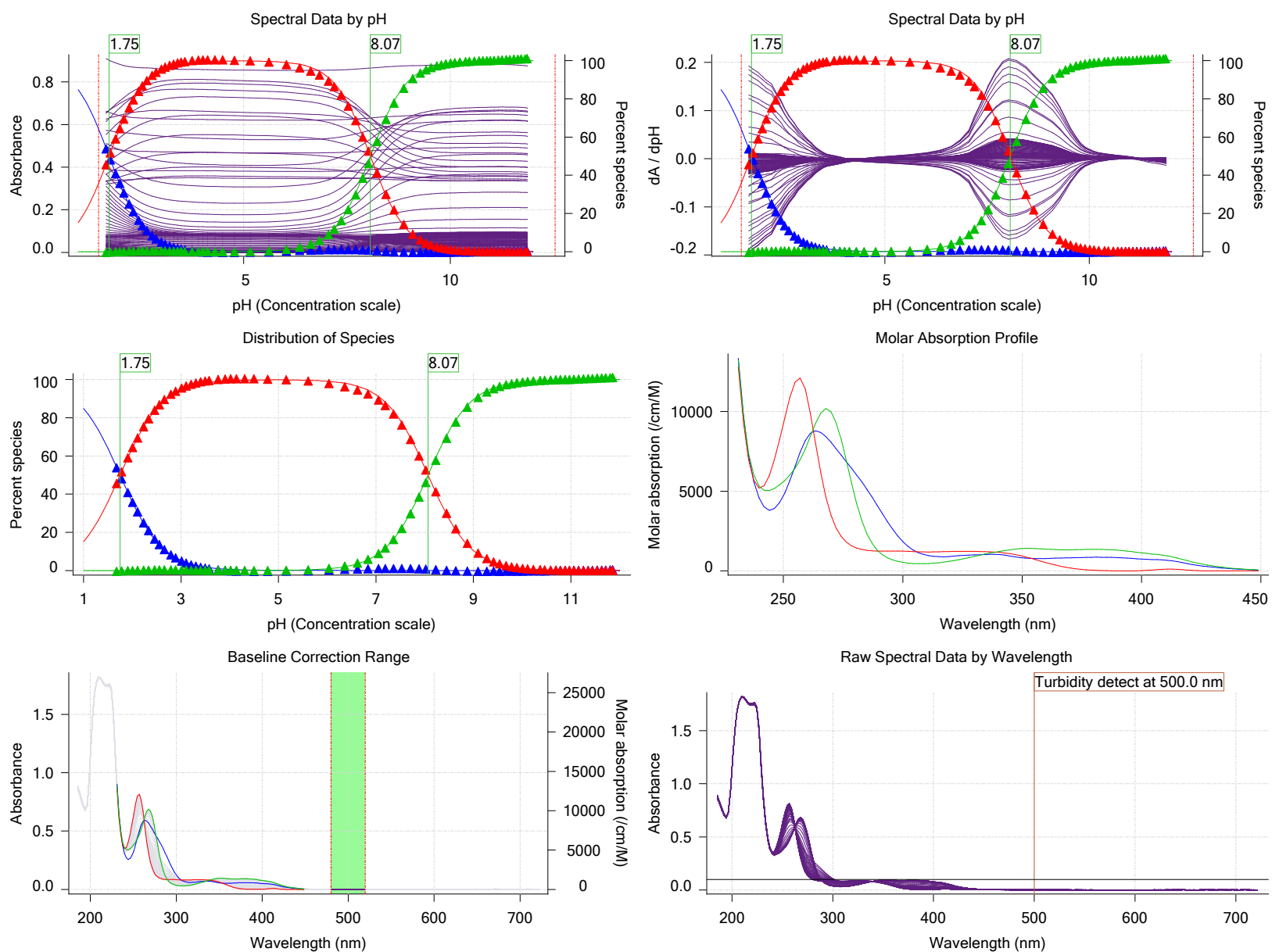
Graphs



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Graphs (continued)



UV-metric psKa Titration 3 of 3 17J-07003 Points 142 to 212

Results

pKa 1 **1.90**
 pKa 2 **7.89**
 RMSD **0.020 0.012 0.023**
 Chi squared **0.1618**
 PCA calculated number of pKas **4**
 Average ionic strength **0.174 M**
 Average temperature **24.9°C**
 Analyte concentration range **57.0 µM to 54.0 µM**
 Methanol weight % **40.1 %**
 Dielectric constant **61.0**
 Water concentration **30.0 M**

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Results (continued)

Number of pKas source **Predicted**
 Wavelength clipping **230.0 nm to 450.0 nm**
 pH clipping **1.497 to 12.522**

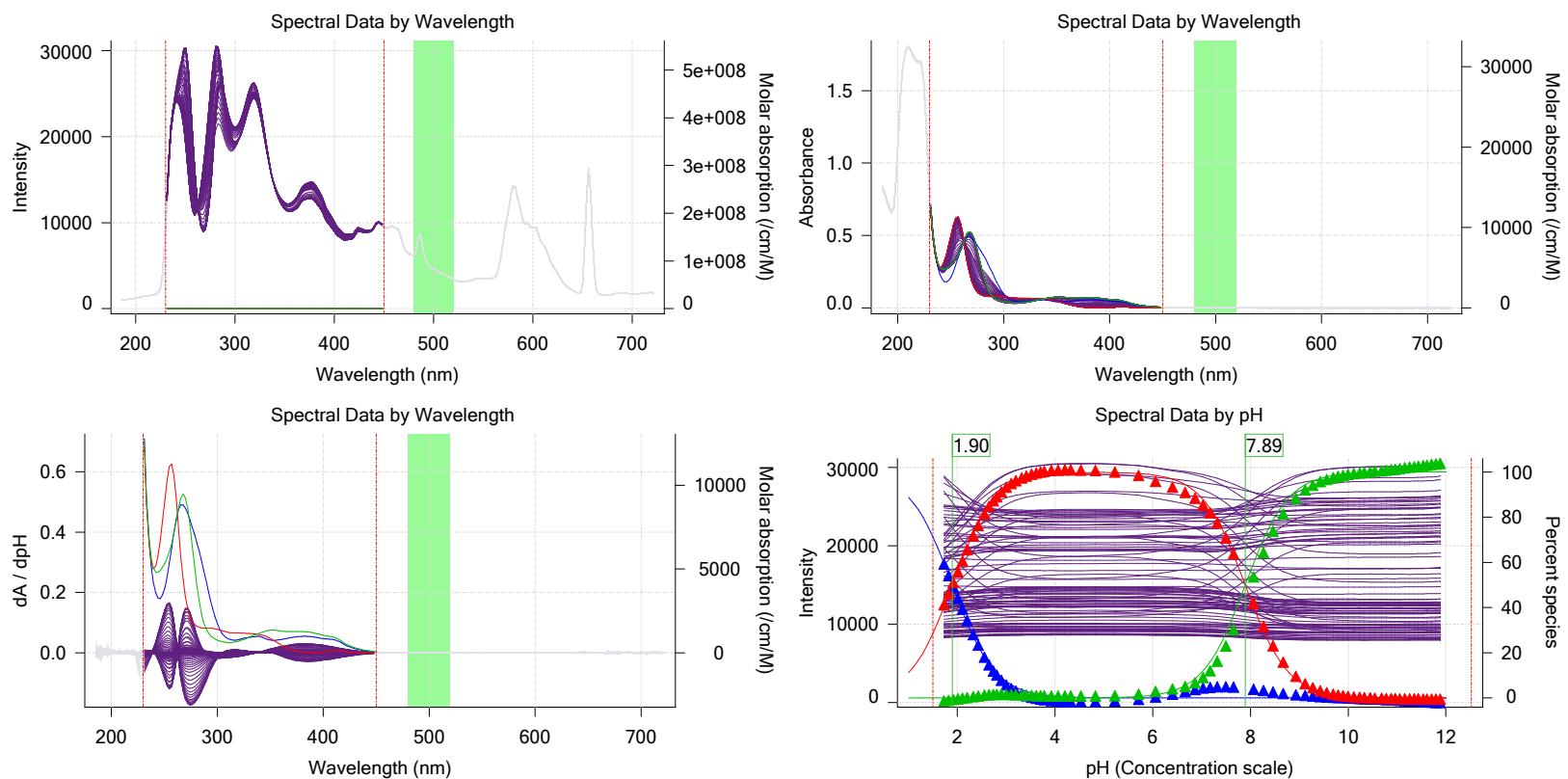
Warnings and errors

Errors None
 Warnings PCA calculation disagrees with predicted number of pKas

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

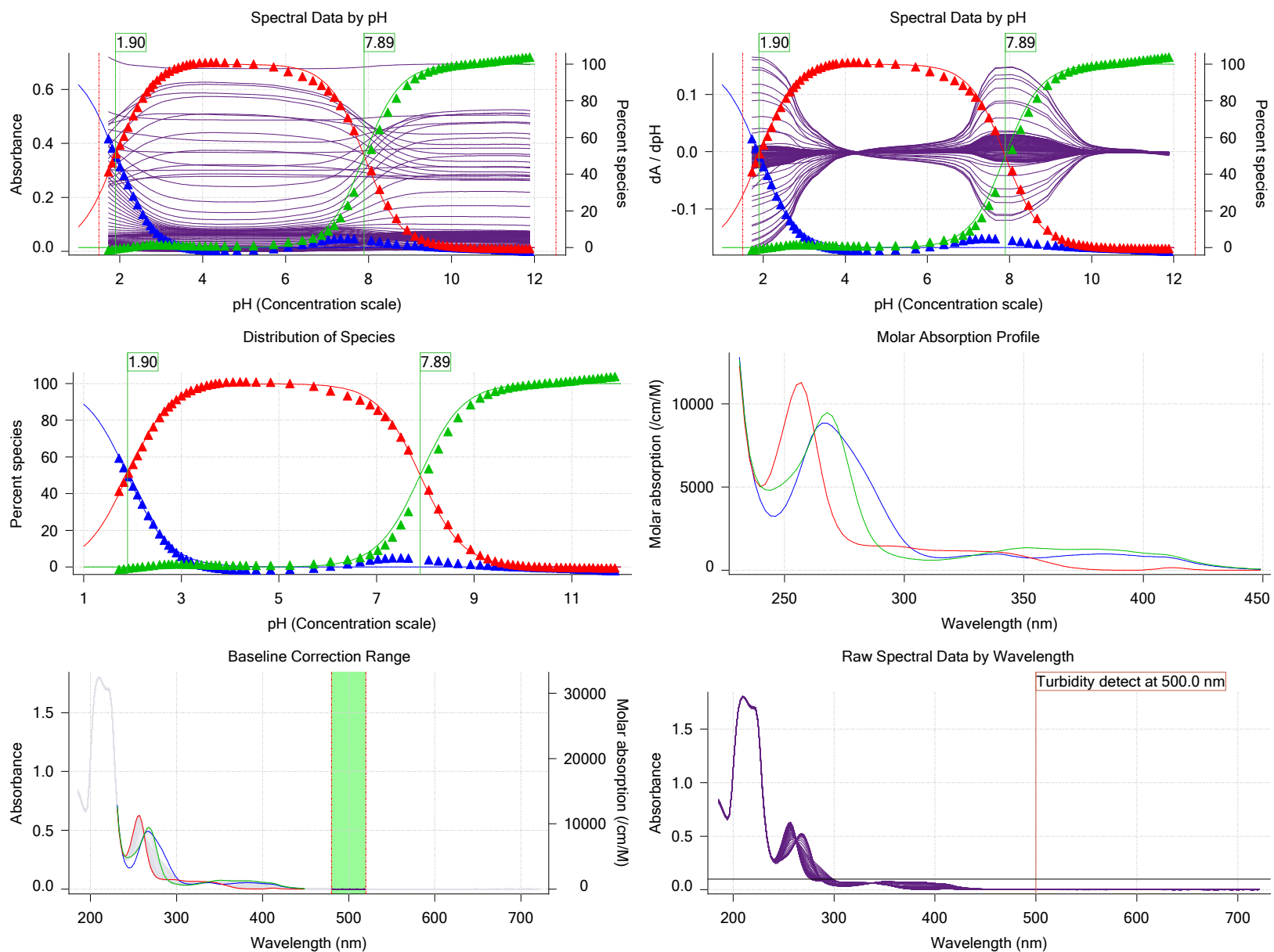
Graphs



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Experiment start time: **10/7/2017 2:51:21 AM**
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Graphs (continued)



Assay Model

Settings

Settings	Value	Date/Time changed	Imported from
Sample name	D07	9/29/2017 6:39:44 PM	User entered value
Sample by	Volume		Default value
Sample volume	0.0040 mL	10/6/2017 6:08:56 PM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.032500 M	10/2/2017 12:59:06 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	396.95	9/29/2017 6:39:58 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	9/29/2017 6:39:44 PM	User entered value
Sample is a	Ampholyte	9/29/2017 6:39:44 PM	User entered value
pKa 1	2.43	9/29/2017 6:39:44 PM	User entered value
Type	Base	9/29/2017 6:39:44 PM	User entered value
pKa 2	7.37	9/29/2017 6:39:44 PM	User entered value
Type	Acid	9/29/2017 6:39:44 PM	User entered value

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Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
logp (XH2 +)	-10.00		Default value
logP (neutral XH)	-10.00	9/29/2017 6:39:44 PM	User entered value
logP (X -)	-10.00		Default value

Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared
3:34.6	Dark spectrum								
3:36.0	Reference spectrum								
4:03.7	Volume reset due to vial change								
5:34.5	Initial pH = 8.37								
6:34.1	Data point 4	0.15005 mL	0.07237 mL	0.00000 mL	1.34995 mL	0.02500 mL	1.962	-0.00317	0.25369
7:02.6	Data point 5	0.15005 mL	0.07237 mL	0.01472 mL	1.34995 mL	0.02500 mL	2.065	0.01126	0.32959
7:19.5	Data point 6	0.15005 mL	0.07237 mL	0.02686 mL	1.34995 mL	0.02500 mL	2.176	-0.00084	0.02202
7:36.2	Data point 7	0.15005 mL	0.07237 mL	0.03652 mL	1.34995 mL	0.02500 mL	2.286	0.00238	0.15010
7:53.0	Data point 8	0.15005 mL	0.07237 mL	0.04405 mL	1.34995 mL	0.02500 mL	2.400	0.00446	0.59254
8:09.7	Data point 9	0.15005 mL	0.07237 mL	0.04988 mL	1.34995 mL	0.02500 mL	2.499	0.00544	0.32949
8:26.3	Data point 10	0.15005 mL	0.07237 mL	0.05456 mL	1.34995 mL	0.02500 mL	2.621	0.00918	0.76769
8:58.5	Data point 11	0.15005 mL	0.07237 mL	0.05903 mL	1.34995 mL	0.02500 mL	2.748	0.00811	0.83437
9:20.3	Data point 12	0.15005 mL	0.07237 mL	0.06096 mL	1.34995 mL	0.02500 mL	2.840	0.00400	0.55029
9:47.1	Data point 13	0.15005 mL	0.07237 mL	0.06286 mL	1.34995 mL	0.02500 mL	2.937	0.00510	0.63912
10:03.7	Data point 14	0.15005 mL	0.07237 mL	0.06458 mL	1.34995 mL	0.02500 mL	3.048	0.00318	0.31187
10:20.4	Data point 15	0.15005 mL	0.07237 mL	0.06592 mL	1.34995 mL	0.02500 mL	3.151	0.00762	0.65884
10:36.9	Data point 16	0.15005 mL	0.07237 mL	0.06698 mL	1.34995 mL	0.02500 mL	3.246	0.00954	0.86684
10:53.5	Data point 17	0.15005 mL	0.07237 mL	0.06783 mL	1.34995 mL	0.02500 mL	3.288	0.01355	0.91245
11:25.5	Data point 18	0.15005 mL	0.07237 mL	0.06872 mL	1.34995 mL	0.02500 mL	3.391	0.01638	0.94484
11:52.3	Data point 19	0.15005 mL	0.07237 mL	0.06933 mL	1.34995 mL	0.02500 mL	3.512	0.02210	0.97013
12:08.9	Data point 20	0.15005 mL	0.07237 mL	0.06978 mL	1.34995 mL	0.02500 mL	3.647	0.02941	0.98104
12:30.6	Data point 21	0.15005 mL	0.07237 mL	0.07037 mL	1.34995 mL	0.02500 mL	3.911	0.05472	0.98729
12:52.3	Data point 22	0.15005 mL	0.07237 mL	0.07070 mL	1.34995 mL	0.02500 mL	4.105	0.07329	0.98190
13:14.0	Data point 23	0.15005 mL	0.07237 mL	0.07088 mL	1.34995 mL	0.02500 mL	4.220	0.09781	0.99184
13:36.5	Data point 24	0.15005 mL	0.07237 mL	0.07103 mL	1.34995 mL	0.02500 mL	4.363	0.09852	0.98299
14:07.9	Data point 25	0.15005 mL	0.07237 mL	0.07114 mL	1.34995 mL	0.02500 mL	4.530	0.10026	0.98953
14:49.2	Data point 26	0.15005 mL	0.07237 mL	0.07124 mL	1.34995 mL	0.02500 mL	4.755	0.09606	0.95170
15:43.9	Data point 27	0.15005 mL	0.07237 mL	0.07131 mL	1.34995 mL	0.02500 mL	5.032	0.10080	0.99573
16:59.3	Data point 28	0.15005 mL	0.07237 mL	0.07138 mL	1.34995 mL	0.02500 mL	5.609	0.19851	0.99794
18:11.0	Data point 29	0.15005 mL	0.07237 mL	0.07143 mL	1.34995 mL	0.02500 mL	6.233	0.25243	0.99796
19:22.7	Data point 30	0.15005 mL	0.07237 mL	0.07147 mL	1.34995 mL	0.02500 mL	6.702	0.09218	0.90876
20:31.9	Data point 31	0.15005 mL	0.07237 mL	0.07154 mL	1.34995 mL	0.02500 mL	7.014	0.09806	0.98464
21:39.2	Data point 32	0.15005 mL	0.07237 mL	0.07161 mL	1.34995 mL	0.02500 mL	7.273	0.09965	0.99156
22:28.0	Data point 33	0.15005 mL	0.07237 mL	0.07168 mL	1.34995 mL	0.02500 mL	7.427	0.09774	0.98478
23:08.3	Data point 34	0.15005 mL	0.07237 mL	0.07175 mL	1.34995 mL	0.02500 mL	7.588	0.10115	0.99721
23:48.1	Data point 35	0.15005 mL	0.07237 mL	0.07183 mL	1.34995 mL	0.02500 mL	7.726	0.09814	0.98887
24:32.0	Data point 36	0.15005 mL	0.07237 mL	0.07192 mL	1.34995 mL	0.02500 mL	7.890	0.09673	0.98571
25:15.4	Data point 37	0.15005 mL	0.07237 mL	0.07201 mL	1.34995 mL	0.02500 mL	8.064	0.10002	0.99100
25:59.3	Data point 38	0.15005 mL	0.07237 mL	0.07211 mL	1.34995 mL	0.02500 mL	8.242	0.09908	0.99608
26:43.6	Data point 39	0.15005 mL	0.07237 mL	0.07220 mL	1.34995 mL	0.02500 mL	8.420	0.09965	0.98377
27:29.5	Data point 40	0.15005 mL	0.07237 mL	0.07230 mL	1.34995 mL	0.02500 mL	8.602	0.09934	0.99251
28:12.9	Data point 41	0.15005 mL	0.07237 mL	0.07239 mL	1.34995 mL	0.02500 mL	8.812	0.09587	0.94273
28:58.0	Data point 42	0.15005 mL	0.07237 mL	0.07248 mL	1.34995 mL	0.02500 mL	9.041	0.09908	0.97329
29:41.2	Data point 43	0.15005 mL	0.07237 mL	0.07255 mL	1.34995 mL	0.02500 mL	9.196	0.09414	0.96176
30:19.5	Data point 44	0.15005 mL	0.07237 mL	0.07262 mL	1.34995 mL	0.02500 mL	9.377	0.09721	0.98050
30:57.8	Data point 45	0.15005 mL	0.07237 mL	0.07270 mL	1.34995 mL	0.02500 mL	9.506	0.09828	0.96689
31:30.1	Data point 46	0.15005 mL	0.07237 mL	0.07277 mL	1.34995 mL	0.02500 mL	9.658	0.09564	0.95662
32:05.5	Data point 47	0.15005 mL	0.07237 mL	0.07286 mL	1.34995 mL	0.02500 mL	9.803	0.09391	0.96750
32:35.8	Data point 48	0.15005 mL	0.07237 mL	0.07295 mL	1.34995 mL	0.02500 mL	9.939	0.09720	0.98468
33:01.1	Data point 49	0.15005 mL	0.07237 mL	0.07305 mL	1.34995 mL	0.02500 mL	10.043	0.09565	0.94953

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 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH S
33:27.9	Data point 50	0.15005 mL	0.07237 mL	0.07317 mL	1.34995 mL	0.02500 mL	10.166	0.07720	0.98213	0.98213
33:54.6	Data point 51	0.15005 mL	0.07237 mL	0.07331 mL	1.34995 mL	0.02500 mL	10.280	0.05739	0.97585	0.97585
34:16.4	Data point 52	0.15005 mL	0.07237 mL	0.07347 mL	1.34995 mL	0.02500 mL	10.394	0.04054	0.97814	0.97814
34:38.1	Data point 53	0.15005 mL	0.07237 mL	0.07366 mL	1.34995 mL	0.02500 mL	10.492	0.03080	0.96824	0.96824
35:04.7	Data point 54	0.15005 mL	0.07237 mL	0.07389 mL	1.34995 mL	0.02500 mL	10.591	0.02015	0.92835	0.92835
35:26.3	Data point 55	0.15005 mL	0.07237 mL	0.07418 mL	1.34995 mL	0.02500 mL	10.695	0.01433	0.92400	0.92400
35:48.0	Data point 56	0.15005 mL	0.07237 mL	0.07455 mL	1.34995 mL	0.02500 mL	10.807	0.00595	0.60447	0.60447
36:09.7	Data point 57	0.15005 mL	0.07237 mL	0.07502 mL	1.34995 mL	0.02500 mL	10.907	0.00411	0.41576	0.41576
36:31.4	Data point 58	0.15005 mL	0.07237 mL	0.07559 mL	1.34995 mL	0.02500 mL	10.999	0.00111	0.04235	0.04235
36:58.3	Data point 59	0.15005 mL	0.07237 mL	0.07700 mL	1.34995 mL	0.02500 mL	11.146	0.00306	0.32740	0.32740
37:30.1	Data point 60	0.15005 mL	0.07237 mL	0.07820 mL	1.34995 mL	0.02500 mL	11.261	-0.00453	0.67584	0.67584
37:57.0	Data point 61	0.15005 mL	0.07237 mL	0.07923 mL	1.34995 mL	0.02500 mL	11.353	-0.00467	0.63841	0.63841
38:13.5	Data point 62	0.15005 mL	0.07237 mL	0.08062 mL	1.34995 mL	0.02500 mL	11.464	-0.00235	0.33895	0.33895
38:30.2	Data point 63	0.15005 mL	0.07237 mL	0.08241 mL	1.34995 mL	0.02500 mL	11.557	-0.00365	0.56650	0.56650
38:46.8	Data point 64	0.15005 mL	0.07237 mL	0.08462 mL	1.34995 mL	0.02500 mL	11.645	-0.00534	0.57589	0.57589
39:03.4	Data point 65	0.15005 mL	0.07237 mL	0.08735 mL	1.34995 mL	0.02500 mL	11.722	-0.00389	0.24919	0.24919
39:30.4	Data point 66	0.15005 mL	0.07237 mL	0.09052 mL	1.34995 mL	0.02500 mL	11.818	-0.00314	0.48821	0.48821
39:47.0	Data point 67	0.15005 mL	0.07237 mL	0.09461 mL	1.34995 mL	0.02500 mL	11.904	-0.00339	0.33145	0.33145
40:03.7	Data point 68	0.15005 mL	0.07237 mL	0.09965 mL	1.34995 mL	0.02500 mL	11.993	-0.00341	0.11203	0.11203
40:20.4	Data point 69	0.15005 mL	0.07237 mL	0.10303 mL	1.34995 mL	0.02500 mL	12.042	-0.00654	0.68141	0.68141
41:55.3	Reference spectrum									
42:57.9	Data point 71	0.22001 mL	0.17237 mL	0.10306 mL	1.34995 mL	0.02500 mL	1.995	-0.03620	0.90558	0.90558
43:25.3	Data point 72	0.22001 mL	0.17237 mL	0.11729 mL	1.34995 mL	0.02500 mL	2.097	0.01250	0.84397	0.84397
43:42.1	Data point 73	0.22001 mL	0.17237 mL	0.12989 mL	1.34995 mL	0.02500 mL	2.221	0.01481	0.89996	0.89996
44:04.1	Data point 74	0.22001 mL	0.17237 mL	0.13791 mL	1.34995 mL	0.02500 mL	2.319	0.00201	0.04028	0.04028
44:31.3	Data point 75	0.22001 mL	0.17237 mL	0.14473 mL	1.34995 mL	0.02500 mL	2.419	0.00710	0.45161	0.45161
44:48.1	Data point 76	0.22001 mL	0.17237 mL	0.15080 mL	1.34995 mL	0.02500 mL	2.543	0.01931	0.94787	0.94787
45:15.3	Data point 77	0.22001 mL	0.17237 mL	0.15503 mL	1.34995 mL	0.02500 mL	2.645	0.01186	0.93909	0.93909
45:31.9	Data point 78	0.22001 mL	0.17237 mL	0.15865 mL	1.34995 mL	0.02500 mL	2.768	0.00845	0.75201	0.75201
45:58.9	Data point 79	0.22001 mL	0.17237 mL	0.16124 mL	1.34995 mL	0.02500 mL	2.860	0.01125	0.91798	0.91798
46:15.4	Data point 80	0.22001 mL	0.17237 mL	0.16345 mL	1.34995 mL	0.02500 mL	2.964	0.00515	0.52568	0.52568
46:32.0	Data point 81	0.22001 mL	0.17237 mL	0.16522 mL	1.34995 mL	0.02500 mL	3.092	0.01000	0.85148	0.85148
46:58.8	Data point 82	0.22001 mL	0.17237 mL	0.16637 mL	1.34995 mL	0.02500 mL	3.189	0.01480	0.89927	0.89927
47:15.4	Data point 83	0.22001 mL	0.17237 mL	0.16740 mL	1.34995 mL	0.02500 mL	3.311	0.01299	0.91139	0.91139
47:42.0	Data point 84	0.22001 mL	0.17237 mL	0.16820 mL	1.34995 mL	0.02500 mL	3.404	0.01010	0.84899	0.84899
47:58.8	Data point 85	0.22001 mL	0.17237 mL	0.16884 mL	1.34995 mL	0.02500 mL	3.507	0.01955	0.95806	0.95806
48:15.3	Data point 86	0.22001 mL	0.17237 mL	0.16933 mL	1.34995 mL	0.02500 mL	3.603	0.01623	0.95327	0.95327
48:31.8	Data point 87	0.22001 mL	0.17237 mL	0.16973 mL	1.34995 mL	0.02500 mL	3.698	0.02643	0.98573	0.98573
48:48.4	Data point 88	0.22001 mL	0.17237 mL	0.17004 mL	1.34995 mL	0.02500 mL	3.787	0.03247	0.98103	0.98103
49:04.9	Data point 89	0.22001 mL	0.17237 mL	0.17030 mL	1.34995 mL	0.02500 mL	3.872	0.04010	0.97518	0.97518
49:26.6	Data point 90	0.22001 mL	0.17237 mL	0.17067 mL	1.34995 mL	0.02500 mL	4.050	0.05652	0.99131	0.99131
49:48.3	Data point 91	0.22001 mL	0.17237 mL	0.17093 mL	1.34995 mL	0.02500 mL	4.194	0.08109	0.99149	0.99149
50:14.9	Data point 92	0.22001 mL	0.17237 mL	0.17114 mL	1.34995 mL	0.02500 mL	4.303	0.08356	0.98509	0.98509
50:36.8	Data point 93	0.22001 mL	0.17237 mL	0.17128 mL	1.34995 mL	0.02500 mL	4.420	0.10028	0.99587	0.99587
51:08.6	Data point 94	0.22001 mL	0.17237 mL	0.17140 mL	1.34995 mL	0.02500 mL	4.590	0.09894	0.99362	0.99362
51:48.3	Data point 95	0.22001 mL	0.17237 mL	0.17150 mL	1.34995 mL	0.02500 mL	4.776	0.10106	0.99749	0.99749
52:36.7	Data point 96	0.22001 mL	0.17237 mL	0.17159 mL	1.34995 mL	0.02500 mL	5.055	0.09968	0.98619	0.98619
53:42.5	Data point 97	0.22001 mL	0.17237 mL	0.17166 mL	1.34995 mL	0.02500 mL	5.430	0.13278	0.99578	0.99578
54:59.2	Data point 98	0.22001 mL	0.17237 mL	0.17173 mL	1.34995 mL	0.02500 mL	5.878	0.13190	0.99307	0.99307
56:15.9	Data point 99	0.22001 mL	0.17237 mL	0.17180 mL	1.34995 mL	0.02500 mL	6.297	0.11466	0.99478	0.99478
57:32.6	Data point 100	0.22001 mL	0.17237 mL	0.17187 mL	1.34995 mL	0.02500 mL	6.618	0.09887	0.99142	0.99142
58:33.4	Data point 101	0.22001 mL	0.17237 mL	0.17194 mL	1.34995 mL	0.02500 mL	6.876	0.10094	0.99357	0.99357
59:31.6	Data point 102	0.22001 mL	0.17237 mL	0.17201 mL	1.34995 mL	0.02500 mL	7.088	0.09921	0.99227	0.99227
1:00:17.9	Data point 103	0.22001 mL	0.17237 mL	0.17211 mL	1.34995 mL	0.02500 mL	7.301	0.09330	0.95086	0.95086
1:00:57.2	Data point 104	0.22001 mL	0.17237 mL	0.17218 mL	1.34995 mL	0.02500 mL	7.439	0.10014	0.99140	0.99140
1:01:38.9	Data point 105	0.22001 mL	0.17237 mL	0.17227 mL	1.34995 mL	0.02500 mL	7.606	0.09813	0.98979	0.98979
1:02:21.9	Data point 106	0.22001 mL	0.17237 mL	0.17244 mL	1.34995 mL	0.02500 mL	7.770	0.09790	0.99627	0.99627

Sample name: **D07**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-07003**
 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 2:51:21 AM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH S
1:03:03.7	Data point 107	0.22001 mL	0.17237 mL	0.17253 mL	1.34995 mL	0.02500 mL	7.949	0.09742	0.98928	0.98928
1:03:46.6	Data point 108	0.22001 mL	0.17237 mL	0.17263 mL	1.34995 mL	0.02500 mL	8.119	0.09898	0.98251	0.98251
1:04:21.9	Data point 109	0.22001 mL	0.17237 mL	0.17269 mL	1.34995 mL	0.02500 mL	8.255	0.09851	0.99305	0.99305
1:05:04.4	Data point 110	0.22001 mL	0.17237 mL	0.17279 mL	1.34995 mL	0.02500 mL	8.458	0.09964	0.99038	0.99038
1:05:52.4	Data point 111	0.22001 mL	0.17237 mL	0.17288 mL	1.34995 mL	0.02500 mL	8.677	0.09820	0.97334	0.97334
1:06:36.2	Data point 112	0.22001 mL	0.17237 mL	0.17295 mL	1.34995 mL	0.02500 mL	8.865	0.09898	0.98259	0.98259
1:07:16.9	Data point 113	0.22001 mL	0.17237 mL	0.17302 mL	1.34995 mL	0.02500 mL	9.096	0.09553	0.96258	0.96258
1:08:00.8	Data point 114	0.22001 mL	0.17237 mL	0.17310 mL	1.34995 mL	0.02500 mL	9.317	0.10068	0.98735	0.98735
1:08:42.0	Data point 115	0.22001 mL	0.17237 mL	0.17317 mL	1.34995 mL	0.02500 mL	9.492	0.09603	0.96675	0.96675
1:09:17.1	Data point 116	0.22001 mL	0.17237 mL	0.17324 mL	1.34995 mL	0.02500 mL	9.632	0.10064	0.98729	0.98729
1:09:49.8	Data point 117	0.22001 mL	0.17237 mL	0.17331 mL	1.34995 mL	0.02500 mL	9.751	0.09893	0.98396	0.98396
1:10:19.7	Data point 118	0.22001 mL	0.17237 mL	0.17340 mL	1.34995 mL	0.02500 mL	9.884	0.09891	0.98270	0.98270
1:10:43.9	Data point 119	0.22001 mL	0.17237 mL	0.17350 mL	1.34995 mL	0.02500 mL	9.994	0.09691	0.96615	0.96615
1:11:06.1	Data point 120	0.22001 mL	0.17237 mL	0.17359 mL	1.34995 mL	0.02500 mL	10.102	0.07482	0.98156	0.98156
1:11:22.7	Data point 121	0.22001 mL	0.17237 mL	0.17368 mL	1.34995 mL	0.02500 mL	10.216	0.05591	0.97990	0.97990
1:11:39.1	Data point 122	0.22001 mL	0.17237 mL	0.17380 mL	1.34995 mL	0.02500 mL	10.319	0.04210	0.96595	0.96595
1:11:55.7	Data point 123	0.22001 mL	0.17237 mL	0.17397 mL	1.34995 mL	0.02500 mL	10.437	0.01994	0.96637	0.96637
1:12:17.4	Data point 124	0.22001 mL	0.17237 mL	0.17422 mL	1.34995 mL	0.02500 mL	10.573	0.00987	0.87943	0.87943
1:12:44.2	Data point 125	0.22001 mL	0.17237 mL	0.17453 mL	1.34995 mL	0.02500 mL	10.665	0.00483	0.45081	0.45081
1:13:00.8	Data point 126	0.22001 mL	0.17237 mL	0.17488 mL	1.34995 mL	0.02500 mL	10.783	0.00177	0.11866	0.11866
1:13:32.6	Data point 127	0.22001 mL	0.17237 mL	0.17549 mL	1.34995 mL	0.02500 mL	10.893	-0.00141	0.09861	0.09861
1:13:59.5	Data point 128	0.22001 mL	0.17237 mL	0.17608 mL	1.34995 mL	0.02500 mL	10.983	-0.00165	0.17162	0.17162
1:14:16.0	Data point 129	0.22001 mL	0.17237 mL	0.17681 mL	1.34995 mL	0.02500 mL	11.080	-0.00431	0.51872	0.51872
1:14:32.6	Data point 130	0.22001 mL	0.17237 mL	0.17773 mL	1.34995 mL	0.02500 mL	11.164	-0.00259	0.37464	0.37464
1:14:59.4	Data point 131	0.22001 mL	0.17237 mL	0.17907 mL	1.34995 mL	0.02500 mL	11.256	-0.00503	0.69652	0.69652
1:15:26.4	Data point 132	0.22001 mL	0.17237 mL	0.18097 mL	1.34995 mL	0.02500 mL	11.352	-0.00558	0.60743	0.60743
1:15:53.4	Data point 133	0.22001 mL	0.17237 mL	0.18288 mL	1.34995 mL	0.02500 mL	11.446	-0.00454	0.68900	0.68900
1:16:10.0	Data point 134	0.22001 mL	0.17237 mL	0.18502 mL	1.34995 mL	0.02500 mL	11.544	-0.00521	0.54566	0.54566
1:16:26.7	Data point 135	0.22001 mL	0.17237 mL	0.18770 mL	1.34995 mL	0.02500 mL	11.629	-0.00375	0.36915	0.36915
1:16:53.9	Data point 136	0.22001 mL	0.17237 mL	0.19156 mL	1.34995 mL	0.02500 mL	11.723	-0.00627	0.69405	0.69405
1:17:20.7	Data point 137	0.22001 mL	0.17237 mL	0.19591 mL	1.34995 mL	0.02500 mL	11.818	-0.00407	0.56951	0.56951
1:17:37.4	Data point 138	0.22001 mL	0.17237 mL	0.20103 mL	1.34995 mL	0.02500 mL	11.895	-0.00193	0.24057	0.24057
1:18:04.6	Data point 139	0.22001 mL	0.17237 mL	0.20783 mL	1.34995 mL	0.02500 mL	11.989	-0.00263	0.47878	0.47878
1:18:21.3	Data point 140	0.22001 mL	0.17237 mL	0.21235 mL	1.34995 mL	0.02500 mL	12.039	-0.00584	0.60456	0.60456
1:20:03.4	Reference spectrum									
1:21:23.7	Data point 142	0.39005 mL	0.29857 mL	0.21237 mL	1.34995 mL	0.02500 mL	1.997	-0.05261	0.96918	0.96918
1:21:45.8	Data point 143	0.39005 mL	0.29857 mL	0.22683 mL	1.34995 mL	0.02500 mL	2.091	0.01063	0.84683	0.84683
1:22:07.9	Data point 144	0.39005 mL	0.29857 mL	0.23798 mL	1.34995 mL	0.02500 mL	2.185	0.00938	0.42022	0.42022
1:22:29.9	Data point 145	0.39005 mL	0.29857 mL	0.24699 mL	1.34995 mL	0.02500 mL	2.276	0.00648	0.27027	0.27027
1:22:51.9	Data point 146	0.39005 mL	0.29857 mL	0.25421 mL	1.34995 mL	0.02500 mL	2.369	0.01077	0.81160	0.81160
1:23:18.8	Data point 147	0.39005 mL	0.29857 mL	0.26065 mL	1.34995 mL	0.02500 mL	2.466	0.00949	0.87743	0.87743
1:23:35.4	Data point 148	0.39005 mL	0.29857 mL	0.26663 mL	1.34995 mL	0.02500 mL	2.588	0.01036	0.88790	0.88790
1:24:02.4	Data point 149	0.39005 mL	0.29857 mL	0.27081 mL	1.34995 mL	0.02500 mL	2.688	0.00637	0.72041	0.72041
1:24:19.1	Data point 150	0.39005 mL	0.29857 mL	0.27441 mL	1.34995 mL	0.02500 mL	2.813	0.00903	0.75955	0.75955
1:24:46.1	Data point 151	0.39005 mL	0.29857 mL	0.27693 mL	1.34995 mL	0.02500 mL	2.909	0.00426	0.47875	0.47875
1:25:18.5	Data point 152	0.39005 mL	0.29857 mL	0.27909 mL	1.34995 mL	0.02500 mL	2.996	0.00319	0.38398	0.38398
1:25:35.1	Data point 153	0.39005 mL	0.29857 mL	0.28086 mL	1.34995 mL	0.02500 mL	3.060	0.00886	0.78262	0.78262
1:25:56.8	Data point 154	0.39005 mL	0.29857 mL	0.28215 mL	1.34995 mL	0.02500 mL	3.155	0.01045	0.87755	0.87755
1:26:23.7	Data point 155	0.39005 mL	0.29857 mL	0.28309 mL	1.34995 mL	0.02500 mL	3.257	0.00522	0.63048	0.63048
1:26:50.6	Data point 156	0.39005 mL	0.29857 mL	0.28387 mL	1.34995 mL	0.02500 mL	3.356	0.01107	0.93400	0.93400
1:27:17.6	Data point 157	0.39005 mL	0.29857 mL	0.28455 mL	1.34995 mL	0.02500 mL	3.450	0.01542	0.86338	0.86338
1:27:34.1	Data point 158	0.39005 mL	0.29857 mL	0.28516 mL	1.34995 mL	0.02500 mL	3.567	0.01197	0.90756	0.90756
1:28:01.0	Data point 159	0.39005 mL	0.29857 mL	0.28565 mL	1.34995 mL	0.02500 mL	3.661	0.01862	0.95448	0.95448
1:28:17.5	Data point 160	0.39005 mL	0.29857 mL	0.28603 mL	1.34995 mL	0.02500 mL	3.768	0.02292	0.97802	0.97802
1:28:34.1	Data point 161	0.39005 mL	0.29857 mL	0.28631 mL	1.34995 mL	0.02500 mL	3.859	0.02973	0.97889	0.97889
1:28:50.6	Data point 162	0.39005 mL	0.29857 mL	0.28655 mL	1.34995 mL	0.02500 mL	3.945	0.03108	0.96810	0.96810
1:29:07.1	Data point 163	0.39005 mL	0.29857 mL	0.28674 mL	1.34995 mL	0.02500 mL	4.024	0.03775	0.97611	0.97611

Sample name: **D07**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-07003**
 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 2:51:21 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
1:29:28.8	Data point 164	0.39005 mL	0.29857 mL	0.28697 mL	1.34995 mL	0.02500 mL	4.164	0.05879	0.98975	0.0029
1:29:50.4	Data point 165	0.39005 mL	0.29857 mL	0.28716 mL	1.34995 mL	0.02500 mL	4.301	0.08405	0.97612	0.0042
1:30:17.1	Data point 166	0.39005 mL	0.29857 mL	0.28730 mL	1.34995 mL	0.02500 mL	4.440	0.09859	0.98587	0.0049
1:30:42.3	Data point 167	0.39005 mL	0.29857 mL	0.28739 mL	1.34995 mL	0.02500 mL	4.562	0.09992	0.98719	0.0049
1:31:16.6	Data point 168	0.39005 mL	0.29857 mL	0.28749 mL	1.34995 mL	0.02500 mL	4.765	0.09955	0.98099	0.0049
1:31:59.5	Data point 169	0.39005 mL	0.29857 mL	0.28758 mL	1.34995 mL	0.02500 mL	5.059	0.09922	0.98040	0.0049
1:32:54.7	Data point 170	0.39005 mL	0.29857 mL	0.28765 mL	1.34995 mL	0.02500 mL	5.452	0.10011	0.98504	0.0049
1:33:59.6	Data point 171	0.39005 mL	0.29857 mL	0.28775 mL	1.34995 mL	0.02500 mL	5.932	0.09917	0.99271	0.0049
1:35:11.5	Data point 172	0.39005 mL	0.29857 mL	0.28782 mL	1.34995 mL	0.02500 mL	6.275	0.09977	0.97803	0.0049
1:36:10.9	Data point 173	0.39005 mL	0.29857 mL	0.28791 mL	1.34995 mL	0.02500 mL	6.617	0.09856	0.99153	0.0048
1:37:00.2	Data point 174	0.39005 mL	0.29857 mL	0.28801 mL	1.34995 mL	0.02500 mL	6.870	0.09994	0.99323	0.0049
1:37:43.0	Data point 175	0.39005 mL	0.29857 mL	0.28810 mL	1.34995 mL	0.02500 mL	7.073	0.09566	0.98828	0.0047
1:38:20.5	Data point 176	0.39005 mL	0.29857 mL	0.28822 mL	1.34995 mL	0.02500 mL	7.233	0.09883	0.98534	0.0049
1:38:57.3	Data point 177	0.39005 mL	0.29857 mL	0.28834 mL	1.34995 mL	0.02500 mL	7.377	0.09790	0.97920	0.0048
1:39:34.4	Data point 178	0.39005 mL	0.29857 mL	0.28848 mL	1.34995 mL	0.02500 mL	7.524	0.09827	0.98393	0.0048
1:40:15.8	Data point 179	0.39005 mL	0.29857 mL	0.28862 mL	1.34995 mL	0.02500 mL	7.697	0.09793	0.98043	0.0048
1:40:57.3	Data point 180	0.39005 mL	0.29857 mL	0.28876 mL	1.34995 mL	0.02500 mL	7.850	0.09979	0.98171	0.0049
1:41:45.0	Data point 181	0.39005 mL	0.29857 mL	0.28918 mL	1.34995 mL	0.02500 mL	8.260	0.10001	0.99182	0.0049
1:42:26.1	Data point 182	0.39005 mL	0.29857 mL	0.28925 mL	1.34995 mL	0.02500 mL	8.458	0.09931	0.96677	0.0049
1:43:08.4	Data point 183	0.39005 mL	0.29857 mL	0.28932 mL	1.34995 mL	0.02500 mL	8.652	0.09790	0.97894	0.0048
1:43:52.1	Data point 184	0.39005 mL	0.29857 mL	0.28939 mL	1.34995 mL	0.02500 mL	8.856	0.09466	0.96836	0.0047
1:44:40.4	Data point 185	0.39005 mL	0.29857 mL	0.28949 mL	1.34995 mL	0.02500 mL	9.110	0.09498	0.95807	0.0048
1:45:28.3	Data point 186	0.39005 mL	0.29857 mL	0.28958 mL	1.34995 mL	0.02500 mL	9.300	0.09832	0.97764	0.0049
1:46:07.0	Data point 187	0.39005 mL	0.29857 mL	0.28968 mL	1.34995 mL	0.02500 mL	9.457	0.09695	0.96428	0.0048
1:46:41.9	Data point 188	0.39005 mL	0.29857 mL	0.28977 mL	1.34995 mL	0.02500 mL	9.607	0.10029	0.98383	0.0050
1:47:12.1	Data point 189	0.39005 mL	0.29857 mL	0.28986 mL	1.34995 mL	0.02500 mL	9.734	0.09666	0.95866	0.0048
1:47:40.9	Data point 190	0.39005 mL	0.29857 mL	0.28998 mL	1.34995 mL	0.02500 mL	9.864	0.09726	0.97509	0.0048
1:48:08.0	Data point 191	0.39005 mL	0.29857 mL	0.29010 mL	1.34995 mL	0.02500 mL	9.967	0.07318	0.97891	0.0036
1:48:29.6	Data point 192	0.39005 mL	0.29857 mL	0.29024 mL	1.34995 mL	0.02500 mL	10.066	0.04385	0.92217	0.0022
1:48:56.4	Data point 193	0.39005 mL	0.29857 mL	0.29041 mL	1.34995 mL	0.02500 mL	10.167	0.02883	0.79342	0.0016
1:49:17.9	Data point 194	0.39005 mL	0.29857 mL	0.29062 mL	1.34995 mL	0.02500 mL	10.286	0.01558	0.89519	0.0008
1:49:39.5	Data point 195	0.39005 mL	0.29857 mL	0.29087 mL	1.34995 mL	0.02500 mL	10.402	0.01094	0.82769	0.0005
1:50:01.2	Data point 196	0.39005 mL	0.29857 mL	0.29116 mL	1.34995 mL	0.02500 mL	10.496	0.00872	0.85603	0.0004
1:50:17.8	Data point 197	0.39005 mL	0.29857 mL	0.29149 mL	1.34995 mL	0.02500 mL	10.616	0.00055	0.02138	0.0001
1:50:39.4	Data point 198	0.39005 mL	0.29857 mL	0.29191 mL	1.34995 mL	0.02500 mL	10.711	-0.00003	0.00005	0.0002
1:50:56.0	Data point 199	0.39005 mL	0.29857 mL	0.29245 mL	1.34995 mL	0.02500 mL	10.847	-0.00342	0.31328	0.0003
1:51:22.7	Data point 200	0.39005 mL	0.29857 mL	0.29318 mL	1.34995 mL	0.02500 mL	10.939	-0.00425	0.58470	0.0002
1:51:39.3	Data point 201	0.39005 mL	0.29857 mL	0.29410 mL	1.34995 mL	0.02500 mL	11.036	-0.00829	0.88051	0.0004
1:51:55.9	Data point 202	0.39005 mL	0.29857 mL	0.29523 mL	1.34995 mL	0.02500 mL	11.121	-0.00666	0.76426	0.0003
1:52:22.8	Data point 203	0.39005 mL	0.29857 mL	0.29685 mL	1.34995 mL	0.02500 mL	11.212	-0.00656	0.75724	0.0003
1:52:49.8	Data point 204	0.39005 mL	0.29857 mL	0.29946 mL	1.34995 mL	0.02500 mL	11.314	-0.00713	0.74880	0.0004
1:53:16.7	Data point 205	0.39005 mL	0.29857 mL	0.30176 mL	1.34995 mL	0.02500 mL	11.411	-0.00690	0.83867	0.0003
1:53:33.4	Data point 206	0.39005 mL	0.29857 mL	0.30447 mL	1.34995 mL	0.02500 mL	11.506	-0.00927	0.76917	0.0005
1:53:50.2	Data point 207	0.39005 mL	0.29857 mL	0.30785 mL	1.34995 mL	0.02500 mL	11.587	-0.00782	0.83981	0.0004
1:54:17.1	Data point 208	0.39005 mL	0.29857 mL	0.31235 mL	1.34995 mL	0.02500 mL	11.684	-0.00788	0.74468	0.0004
1:54:33.8	Data point 209	0.39005 mL	0.29857 mL	0.31750 mL	1.34995 mL	0.02500 mL	11.759	-0.00891	0.80597	0.0004
1:55:00.8	Data point 210	0.39005 mL	0.29857 mL	0.32406 mL	1.34995 mL	0.02500 mL	11.853	-0.00651	0.66133	0.0004
1:55:17.6	Data point 211	0.39005 mL	0.29857 mL	0.33180 mL	1.34995 mL	0.02500 mL	11.939	-0.00758	0.91302	0.0003
1:55:34.4	Data point 212	0.39005 mL	0.29857 mL	0.34137 mL	1.34995 mL	0.02500 mL	12.022	-0.00881	0.75425	0.0005
1:57:33.6	Assay volumes	0.64005 mL	0.42959 mL	0.34137 mL	1.34995 mL	0.02500 mL				

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Dorothy Levorse			
Separate reference vial	Yes			
Standard Experiment Settings				

Sample name: **D07**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-07003**
 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 2:51:21 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	12.000			
pH step between points of	0.100			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	Spectrometer			
Monitor at a wavelength of	500.0 nm			
Absorbance threshold of	0.100			
Collect turbidity sensor data	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	15%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
Cosolvent in use	Yes			
Cosolvent type	Methanol			
Cosolvent volume	1.35 mL			
Cosolvent added	Automatic			
ISA water volume	0.15 mL			
Water added	Automatic			
After water addition, stir for	5 seconds			
At a speed of	15%			
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			
After medium addition, stir for	5 seconds			
Sample Sonication				
Sonicate	No			
Sample Dissolution				
Perform a dissolution stage	No			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	15%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	10 seconds			
Titration 2				
Titrate from	Low to high pH			
Additional cosolvent volume	0.00 mL			
Add additional water	0.07 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
Titration 3				
Titrate from	Low to high pH			
Additional cosolvent volume	0.00 mL			
Add additional water	0.17 mL			
Additional water added	Automatic			

Sample name: **D07**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-07003**
 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 2:51:21 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
After pH adjust stir for	10 seconds			
Data Point Stability				
Stir during data point collection	Yes			
For point collection, stir at	15%			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00500 dpH/dt			
Stability timeout after	60 seconds			
Experiment cleanup				
Adjust pH to cleanup	To start pH			
And then stir for	60 seconds			
For cleaning, stir at	20%			
Then add water volume	0.25 mL			
And then stir for	30 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.161	10/7/2017 2:51:21 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Four-Plus S	0.9927	10/7/2017 2:51:21 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Four-Plus jH	0.5	10/7/2017 2:51:21 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Four-Plus jOH	-0.7	10/7/2017 2:51:21 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Base concentration factor	1.011	10/7/2017 2:51:21 AM	C:\Sirius_T3\KOH17122.t3r
Acid concentration factor	1.003	10/7/2017 2:51:21 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T311053		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1100253	3/31/2009 6:24:52 AM
Dispenser 0	Water		3/31/2009 6:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	8-18-17	9/26/2017 9:05:04 AM
Dispenser 2	Acid		3/31/2009 6:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	166940 and 172875	10/6/2017 2:55:40 PM
Dispenser 1	Base		3/31/2009 6:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9-22-17	9/22/2017 4:02:42 PM
Dispenser 5	Cosolvent		3/31/2009 6:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 6:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	9-26-17	10/5/2017 5:02:03 PM
Port B	Cyclohexane		9/19/2017 2:15:02 PM
Port C	MeCN (50%, 0.15 M KCl)	10-2-17	10/2/2017 11:28:55 AM
Dispenser 3	Buffer		8/3/2010 6:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Phosphate Buffer		9/12/2017 12:32:29 PM

Sample name: **D07**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-07003**
 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 2:51:21 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Dispenser 6	Octanol		10/22/2010 11:52:43 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titration	Octanol	9-14-17	9/14/2017 10:30:38 AM
Titration		T3TM1100153	3/31/2009 6:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0769	8/15/2017 10:21:54 AM
E0 calibration	-9.13 mV		10/7/2017 2:51:45 AM
Filling solution	3M KCl	KCL095	10/4/2017 3:50:10 PM
Liquids			
Wash 1	50% IPA:50% Water		10/6/2017 2:50:08 PM
Wash 2	0.5% Triton X-100 in H2O		10/6/2017 2:50:11 PM
Buffer position 1	pH7 Wash		10/6/2017 2:50:17 PM
Buffer position 2	pH 7		10/6/2017 2:50:19 PM
Storage position			10/6/2017 2:50:25 PM
Wash water	9e+003 mL	10-6-17	10/6/2017 3:04:25 PM
Waste	1e+003 mL		10/6/2017 3:04:33 PM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		072390	11/23/2010 12:22:28 PM
Dip probe		11086	
Wavelength coefficient A0	185.563		
Wavelength coefficient A1	2.17439		
Wavelength coefficient A2	-0.000285622		
Total lamp lit time	391:10:29		11/23/2010 12:22:28 PM
Calibrated on	10/5/2017 10:23:25 AM		
Integration time	11		
Scans averaged	10		
Autoloader		T3AL1100237	11/10/2015 10:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titration tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		



Assay Settings

Sample name: **D07** Experiment start time: **10/7/2017 2:51:21 AM**
Assay name: **UV-metric psKa** Analyst: **Dorothy Levorse**
Assay ID: **17J-07003** Instrument ID: **T311053**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
E0 calibration reading stir speed	0%		
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	Spectrometer	Spectrometer
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00
Exclude turbid points	Yes	Yes
Low intensity warning threshold	100	100
Minimum absorbance change threshold	0.100	0.100
Eigenvector autocorrelation threshold	0.80	0.80
Maximum RMSD severe warning	0.250	0.250
Maximum RMSD warning	0.050	0.050

Tray Information

Title
Location F1